

Quantum phase transitions of the spin-boson model within multi-coherent-states

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A variational approach based on the multi-coherent-state ansatz with asymmetric parameters is employed to study the ground state of the spin-boson model. Without any artificial approximations except for the finite number of the coherent states, we find the robust Gaussian critical behavior in the whole sub-Ohmic bath regime. The converged critical coupling strength can be estimated with the $1/N$ scaling, where N is the number of the coherent states. It is strongly demonstrated the breakdown of the well-known quantum-to-classical mapping for $1/2 < s < 1$. In addition, the entanglement entropy displays more steep jump around the critical points for the Ohmic bath than the sub-Ohmic bath.

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I. INTRODUCTION

A quantum system inevitably couples to the environmental degree of freedom, which forms an open quantum system [1]. It is of great significance to understand the influence of environment on the quantum system. As a paradigmatic model to study the open quantum systems, the spin-boson model has drawn persistent attentions [2]. In the spin-boson model, the quantum system is simplified as a single spin (qubit), while the environment is abstracted into a bosonic bath with an infinite number of modes. The coupling between the qubit and the environment is characterized by a spectral function $J(\omega)$ which is proportional to ω^s . The spectral exponent s varies the spin-boson model into three different types: sub-Ohmic ($s < 1$), Ohmic ($s = 1$), and super-Ohmic ($s > 1$).

Despite its simple form, there still exist great challenges to analyze the spin-boson model, due to the continuous bosonic bath which leads to an infinite number of degree of freedoms. The difficulties are aggravated by the infrared divergence of the sub-Ohmic and Ohmic spin-boson model which has close relations with the quantum phase transition (QPT) [2–5]. Many advanced numerical approaches have been applied to this model, such as the numerical renormalization group (NRG) [6–8], quantum Monte Carlo simulation (QMC) [9], sparse polynomial space approach [10], exact diagonalization in terms of shift boson [11], and variational matrix product state method [12, 13]. It is generally accepted that there exists a second-order QPT for sub-Ohmic baths and the Kosterlitz-Thouless QPT for the Ohmic bath.

It has been argued for a long time that the QPT of the present quantum model is in the same universality class as the thermodynamic phase transition of the one-dimensional Ising model with long-range interactions [1, 14–16]. This quantum-to-classical correspondence was supported by most numerical approaches, but also questioned by a Berry phase term emerged in the action [17, 18]. Most recently, we have developed a displaced Fock State (DFS) method [19] to analytically study the sub-Ohmic spin-boson model and present evi-

dence of the Gaussian criticality persistent in the whole sub-Ohmic bath regime.

The variational study based on the polaronic unitary transformation by Silbey and Harris [20] has inspired a lot of studies by means of coherent states and various extensions [21–28]. Zheng *et al.* reproduced the results of Silbey-Harris ansatz by unitary transformation without variational procedures. The zeroth-order approximation in DFS method [19] can also recover the famous Silbey-Harris results. A generalized Silbey-Harris ansatz was proposed by Chin *et al.* which correctly describes a continuous transition with mean-field exponents for $0 < s < 1/2$ [22]. However, it failed to give reliable critical points for $1/2 < s < 1$ [26].

Recently, the single coherent states ansatz [20] was improved by simply adding other coherent states on the equal footing [25] and by superpositions of two degenerate single coherent states [26], which are generally termed as multi-coherent-states (MCS) ansatz in this paper. Actually, the MCS in the single-mode version has been proposed ten years before by Ren *et al.* [29] independently. Bera *et al.* [25] have studied the novel environmental entanglement and spin coherence in the Ohmic spin-boson model by increasing the number of the coherent states without much more difficulties. Very interestingly, the MCS ansatz was shown to have fast convergence and can give results with very high accuracy. The variational study using MCS with unconstrained parameters have not been studied in the spin-boson model, which may hopefully shed light on the quantum criticality of the spin-boson model.

Among all single coherent ansatz, any correlations among bosons are not included, so in principle the non-mean-field exponent can not be given. While the correlations among phonons should be certainly embodied in the MCS ansatz. Recently, diagrammatic multiscale methods anchored around local approximations, where the particle correlations are self-consistently taken into account, indeed capture the well known non-mean-field nature of a lattice model [30]. So it is expected that MCS would give the precise description for the quantum

criticality also, which motivate the present study for the QPT in both sub-Ohmic and Ohmic spin-boson model within the MCS ansatz without imposing any limits on the variational parameters.

The rest of paper is organized as follows. In Sec. II, the spin-boson Hamiltonian is introduced briefly. The asymmetrical MCS ansatz is proposed in Sec. III, and the self-consistent equations for the variational parameters are derived. The numerical results for the order parameter and the entanglement entropy are presented and discussed in Sec. IV, and conclusions are given in the last section.

II. HAMILTONIAN

The spin-boson Hamiltonian can be written as

$$\hat{H} = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{\sigma_z}{2} \sum_k \lambda_k (b_k^\dagger + b_k), \quad (1)$$

where σ_i ($i = x, y, z$) are the Pauli matrices, Δ is the tunneling amplitude between the spin-up state $|\uparrow\rangle$ and the spin-down state $|\downarrow\rangle$, b_k (b_k^\dagger) is the bosonic annihilation (creation) operator which can (create) a boson with frequency ω_k , λ_k is the corresponding coupling strength between the qubit and the bosonic bath, which is determined by the spectral density $J(\omega)$,

$$J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k) = 2\alpha\omega_c^{1-s}\omega^s \Theta(\omega_c - \omega), \quad (2)$$

where α is a dimensionless coupling constant, ω_c is the cutoff frequency which is set to be 1 throughout this paper, $\Theta(\omega_c - \omega)$ is a step function.

III. MULTI-COHERENT-STATE ANSATZ

The ground-state in the generalized Silbey-Harris ansatz [22, 23] can be written in the bases of spin-up state $|\uparrow\rangle$ and spin-down state $|\downarrow\rangle$ as

$$|\Psi\rangle = \begin{pmatrix} A \exp \left[\sum_{k=1}^{N_b} f_k (b_k^\dagger - b_k) \right] |0\rangle \\ B \exp \left[\sum_{k=1}^{N_b} g_k (b_k^\dagger - b_k) \right] |0\rangle \end{pmatrix}, \quad (3)$$

where A (B) is related to the occupation probabilities of spin-up (spin-down) state, while f_k (g_k) are the corresponding bosonic displacements of the k th mode. It can be reduced to the original Silbey-Harris ansatz if set $A = B$, and $f_k = -g_k$. Note that the nonlocal correlations among phonons are not included in this ansatz, so non-mean-field nature cannot be described in this ansatz. In the recent analytic DFS method [19], correlations for more than one phonon can be fully considered step by step. This is a very clean and rigorous approach where the correlations among phonons are explicitly shown.

However, even the nearly converged results for the magnetic order parameter up to the third-order DFS still cannot give the non-mean-field nature for $s > 1/2$. Note that in the DFS, the number of the parameters for the self-consistent solutions, which are required in the discretization in the continuous integral, increase exponentially with the approximation order, so it becomes extremely difficult to explore the further corrections.

It is very interesting to note that the correlations among more phonons can be also included in the MCS ansatz [25, 29]. More importantly, the number of variational parameters only increases with the number of the coherent states linearly, so the high order of approximations can be practically performed. It is expected that the MCS can provide insights upon the nontrivial critical behavior of the spin-boson model.

A general form of the MCS in the bases of spin-up state $|\uparrow\rangle$ and spin-down state $|\downarrow\rangle$ can be written as

$$|\Psi\rangle = \begin{pmatrix} \sum_{n=1}^N A_n \exp \left[\sum_{k=1}^{N_b} f_{n,k} (b_k^\dagger - b_k) \right] |0\rangle \\ \sum_{n=1}^N B_n \exp \left[\sum_{k=1}^{N_b} g_{n,k} (b_k^\dagger - b_k) \right] |0\rangle \end{pmatrix}, \quad (4)$$

where A_n (B_n) are related to the occupation probabilities of spin-up (spin-down) state, while $f_{n,k}$ ($g_{n,k}$) are the corresponding bosonic displacements of the k th mode, and $|0\rangle$ is the vacuum state of the bosonic bath. N is the number of the coherent states, and N_b is the number of the discrete bosonic modes. A generalized Silbey-Harris ansatz [22] can thus be recovered if set $N = 1$. The symmetric MCS ansatz ($A_n = B_n$ and $f_{n,k} = -g_{n,k}$) can only be applied to the delocalized phase. In the spin-boson model, since the QPT may occur with a symmetry breaking, the asymmetric wavefunction 4) should be generally employed.

The energy expectation value can be expressed as

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (5)$$

where

$$\begin{aligned} \langle \Psi | \hat{H} | \Psi \rangle &= \sum_{m,n} (A_m A_n F_{m,n} \alpha_{m,n} \\ &\quad + B_m B_n G_{m,n} \beta_{m,n} - \Delta \Gamma_{m,n} A_m B_n), \\ \langle \Psi | \Psi \rangle &= \sum_{m,n} (A_m A_n F_{m,n} + B_m B_n G_{m,n}), \end{aligned}$$

with

$$\begin{aligned}
F_{m,n} &= \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - f_{n,k})^2 \right], \\
G_{m,n} &= \exp \left[-\frac{1}{2} \sum_k (g_{m,k} - g_{n,k})^2 \right], \\
\Gamma_{m,n} &= \exp \left[-\frac{1}{2} \sum_k (f_{m,k} - g_{n,k})^2 \right], \\
\alpha_{m,n} &= \sum_k \left[\omega_k f_{m,k} f_{n,k} + \frac{\lambda_k}{2} (f_{m,k} + f_{n,k}) \right], \\
\beta_{m,n} &= \sum_k \left[\omega_k g_{m,k} g_{n,k} - \frac{\lambda_k}{2} (g_{m,k} + g_{n,k}) \right].
\end{aligned}$$

The parameters $\{A_n\}$, $\{B_n\}$, $\{f_{n,k}\}$, and $\{g_{n,k}\}$ are determined by minimizing the energy expectation value E with respect to the variational parameters. The total number of variational parameters is $2N(N_b + 1)$. For A_n and B_n , we have

$$\sum_n (2A_n F_{i,n} (\alpha_{i,n} - E) - \Gamma_{i,n} B_n \Delta) = 0, \quad (6)$$

$$\sum_n (2B_n G_{i,n} (\beta_{i,n} - E) - \Gamma_{n,i} A_n \Delta) = 0, \quad (7)$$

and for $f_{n,k}$ and $g_{n,k}$, we obtain

$$\begin{aligned}
&\sum_n \{ -\Delta \Gamma_{i,n} B_n g_{n,k} \\
&+ A_n F_{i,n} [2(\alpha_{i,n} + \omega_k - E) f_{n,k} + \lambda_k] \} = 0, \quad (8)
\end{aligned}$$

$$\begin{aligned}
&\sum_n \{ -\Delta \Gamma_{n,i} A_n f_{n,k} \\
&+ B_n G_{i,n} [2(\beta_{i,n} + \omega_k - E) g_{n,k} - \lambda_k] \} = 0. \quad (9)
\end{aligned}$$

In practise, these parameters can be obtained by solving the coupled equations self-consistently, which in turn give the GS energy and wavefunction. Generally, the largest number of the coherent states in the practical calculations can be reached up to $N_{\max} = 10$ in this paper.

In the DFS study [19], we have rigourously proved that all summation over k is related to $\sum_k \lambda_k^2$, and can be transformed into the continuous integral $\int_0^{\omega_c} d\omega J(\omega) I(\omega)$. To be free from any approximation except for the finite number of the MCS, the exact summation over k should be performed. We here use the Gaussian-logarithmical discretization developed in Ref. [19] to calculate the continuous spectral numerically exactly by checking the convergence. The widely used logarithmical discretization usually overestimate the critical points [19].

In order to check the validity of the MCS ansatz with unconstrained the parameters, we compare the ground state energy calculated by Eq. (5) for the different number of coherent states (N). We present the relative difference $\delta E_N = (E_N - E_{N_{\max}})/E_{N_{\max}}$ as a function

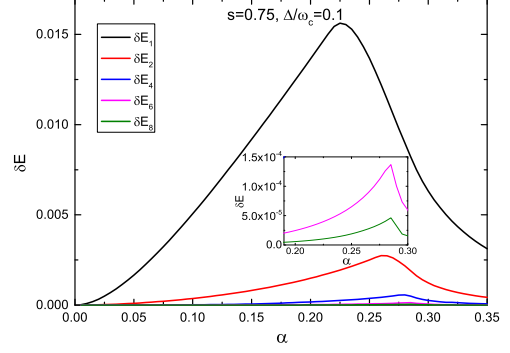


FIG. 1: (Color online) The ground state energy relative difference $\delta E_N = (E_N - E_{10})/E_{10}$ as a function of α for various numbers of coherent states. The inset is an enlarged view for $N = 6$ and 8 curves. $s = 0.75$ and $\Delta/\omega_c = 0.1$.

of the coupling strength α in Fig. 1 for $s = 0.75$ and $\Delta/\omega_c = 0.1$. It is shown that δE_N becomes smaller rapidly with increasing N . δE_{10} is always less than 10^{-5} in the whole coupling regime, demonstrating that an excellent convergence is achieved for $N_{\max} = 10$. In other words, $N_{\max} = 10$ is sufficient large to describe the ground-state in this model. In the next section, we will study the criticality of the spin-boson model with the MCS by using the numerically exact Gaussian-logarithmical integrations.

IV. RESULTS AND DISCUSSIONS

It is well-known that the magnetization M acts as an order parameter in the sub-Ohmic spin-boson model, which can be written as

$$M = \frac{\langle \Psi | \sigma_z | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{1}{D} \sum_{m,n} (A_m A_n F_{m,n} - B_m B_n G_{m,n}). \quad (10)$$

Figure. 2 shows the value of M as a function of α for different numbers of coherent states. It is obvious that there exists a critical coupling strength α_c which separates the delocalized phase with zero magnetization from the localized one with nonzero magnetization. In the weak coupling regime, the magnetization M is always zero, indicating that the spin stay in the spin-up and the spin-down states with the same probability. With increasing coupling strength, M will tend to 1 (due to the degeneracy, another branch will tend to -1 symmetrically). The critical coupling strength α_c increases with the value of s , as shown in Fig. 2. For same spectral exponent s , the obtained α_c increases with the number of coherent state. The Ohmic case was studied by the symmetric MCS ansatz for $0 < \alpha < 1$ in Ref. [25]. It should be noted that the symmetric MCS is invalid in the localized phase.

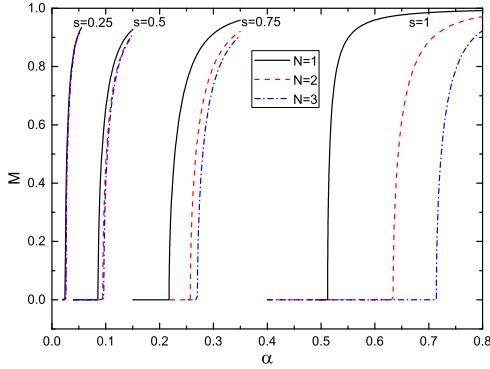


FIG. 2: (Color online) The magnetization M as a function of α for $s = 0.25, 0.5, 0.75$, and 1 with $N = 1, 2$, and 3 . $\Delta/\omega_c = 0.1$.

We then pay particular attention to $s = 0.75$, which is typical value greater than 0.5 . As shown in Fig. 3, a fast convergence for the magnetization can be achieved with increasing number of the coherent states. In principle, the true critical coupling strength α_c should only be obtained by the infinite number of the coherent states in the MCS, which definitely cannot be realized in the practical calculations. It also becomes extremely difficult to solve the self-consistent equations [6]-[9] for an unbounded large number of coherent states, especially near critical points. Fortunately, a perfect linear scaling α_c as a function of the inverse coherent state number $1/N$ is shown in the inset of Fig. 3. In this way, α_c is extrapolated to 0.2952 when $1/N \rightarrow 0$, i.e. $N \rightarrow \infty$. Very interestingly, this value for α_c is consistent excellently with 0.2951 obtained by QMC [9], the only numerical method where the discretization of the bath is not needed in literature, to the best of our knowledge.

The magnetization shows a power law behavior near the critical point, namely $M \propto (\alpha - \alpha_c)^\beta$. The classical counterpart of the sub-Ohmic spin-boson model is the one-dimensional Ising model with long-range interaction according to the quantum-to-classical mapping [1, 14, 15]. It is predicted that a continuous phase transition with mean-field behavior undergoes for $0 < s < 1/2$ and non-mean-field behavior for $1/2 < s < 1$. Most previous numerical approaches demonstrated the validity of the quantum-to-classical mapping. Surprisingly, the DFS method [19] gives the robust mean-field exponent $\beta = 1/2$ in the whole sub-Ohmic regime $0 < s < 1$, which is in sharp contrast with the previous conclusions. Therefore, the critical behavior of the sub-Ohmic spin-boson model needs further extensive direct studies where the Berry phase and topological effects are not missed [17, 18]. The studies based on the Feynman path-integral representation of the partition function may not satisfy this requirement.

Figure. 4 displays the log-log plot of magnetization as

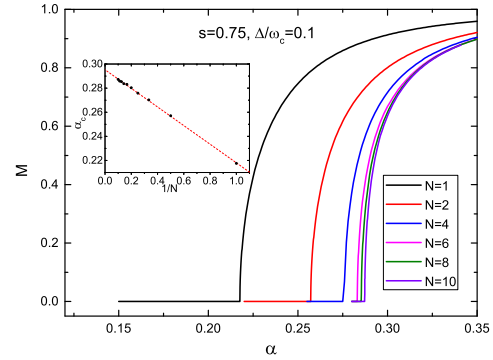


FIG. 3: (Color online) The magnetization M as a function of α with seven numbers of coherent states for $s = 0.75$ and $\Delta/\omega_c = 0.1$. Inset shows the critical coupling strength α_c as a function of the inverse coherent state number $1/N$. A very nice linear fitting yields the extrapolated limiting value $\alpha_c = 0.2952$ as $N \rightarrow \infty$.

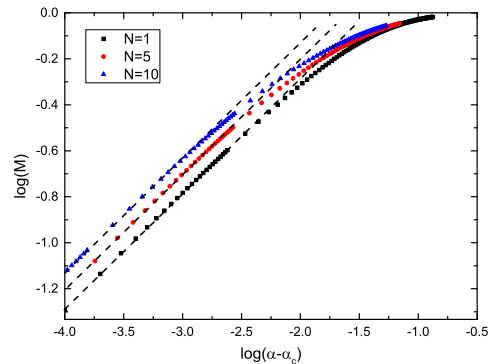


FIG. 4: (Color online) Log-log plot of magnetization M as a function of $(\alpha - \alpha_c)$ for $s = 0.75$ and $\Delta/\omega_c = 0.1$ with the number of coherent state $N = 1$ (square), 5 (cycle) and 10 (triangle). The power law curves with $\beta = 0.5$ is denoted by the dashed line.

a function of $(\alpha - \alpha_c)$ for $s = 0.75$ for $N = 1, 5$, and 10 . It is surprising to observe that all curves show a very nice power-law behavior over more than 2 decades with an exponent $\beta = 0.5$. It is strongly suggested that even $N = 10$ coherent states can hardly modify the exponent β . In other words, the number of coherent state N has negligible effect on the critical exponent $\beta \sim 1/2$, unlike the critical coupling strength α_c which is quite sensitive on N . So here we provide another piece of evidence for the breakdown of the quantum-to-classical mapping for $1/2 < s < 1$, besides the DFS study [19].

Now we move to the Ohmic bath case ($s = 1$). To demonstrate the difference between the $s = 1$ and $s < 1$ baths, we study the entanglement entropy between the qubit and the bath. In the spin-boson model, entangle-

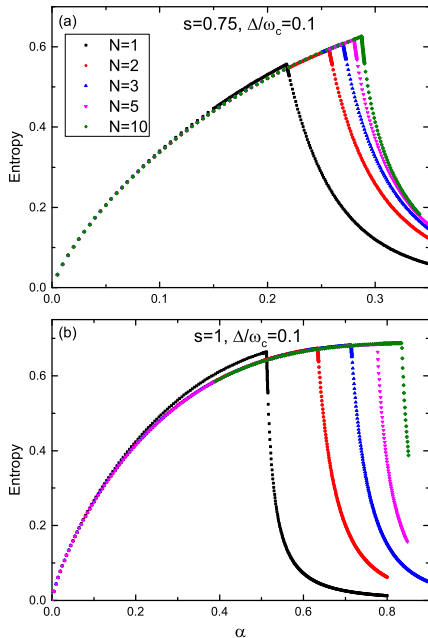


FIG. 5: (Color online) The entanglement entropy as a function of the coupling strength for $s = 0.75$ (a) and $s = 1$ (b).

ment entropy can be obtained as [4]

$$S = -p_+ \log p_+ - p_- \log p_-,$$

where $p_{\pm} = (1 \pm \sqrt{\langle \sigma_x \rangle^2 + \langle \sigma_z \rangle^2})/2$. In the exact NRG study [5], $-\langle \sigma_x \rangle = \Delta/\omega_c$ for $\alpha \rightarrow 1$. So in the delocalized phase, the entanglement entropy should converge to $S \simeq \ln 2 - \frac{\langle \sigma_x \rangle^2}{\ln 10}$ at the strong coupling, which is 0.6888 for $\Delta/\omega_c = 0.1$.

The entanglement entropy as a function of the coupling strength is given in Fig. 5 for $s = 0.75$ and $s = 1$ at $\Delta/\omega_c = 0.1$. We observe that the entanglement entropy exhibits a cusp for $s < 1$, and shows a very steep drop for $s = 1$ at the critical points. With increase of the number of the coherent states, the entanglement entropy jump more steeply at the critical point. Interestingly, the entanglement entropy curves for $s = 1$ resemble very

much curves for unbiased case in Fig. 4 of Ref. [5] by the Bethe ansatz study at extremely low temperature. It is expected that the entanglement entropy will vertically jump to zero in the limit of $N \rightarrow \infty$. This may be a signature of the Kosterlitz-Thouless type QPT from a second-order QPT. The Kosterlitz-Thouless phase transition, of infinite order, for the Ohmic bath ($s = 1$) [1, 2], can be only reached in the infinite number of coherent states. Such a sudden jump is not, but perhaps related to the sudden jump of the superfluid density in thin films of He^4 described by the two-dimensional XY model [31], which is worthy of a further study.

V. CONCLUSION

In this work, by means of the asymmetric MCS ansatz, we extensively analyze the ground state of the spin-boson model, especially the quantum criticality. This direct study to the quantum model does not miss the Berry phase or topological defects. Without any artificial approximations except for the finite number of the coherent states, we find that the magnetic exponent $\beta \sim 1/2$ at the critical points is robust in the whole sub-Ohmic bath regime, consistent with the recent DFS study and in contrast with most numerical studies in literature. It is strongly suggested that the well-known quantum-to-classical mapping is broken down for $1/2 < s < 1$. The asymptotical behavior in the infinite number of the coherent states are also analyzed. The converged critical strengths for $s = 0.75$ agrees well with the QMC formulated on Feynman path-integral representation of the partition function. For $s = 1$, more steep jump of the entanglement entropy at the critical point for the larger number N of the coherent states is observed. It is expected that the vertical jump of the entanglement entropy would occur at the Kosterlitz-Thouless phase transition points in the large N limit.

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